Multiscale Materials Design

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Conference on Fossil Energy
Materials

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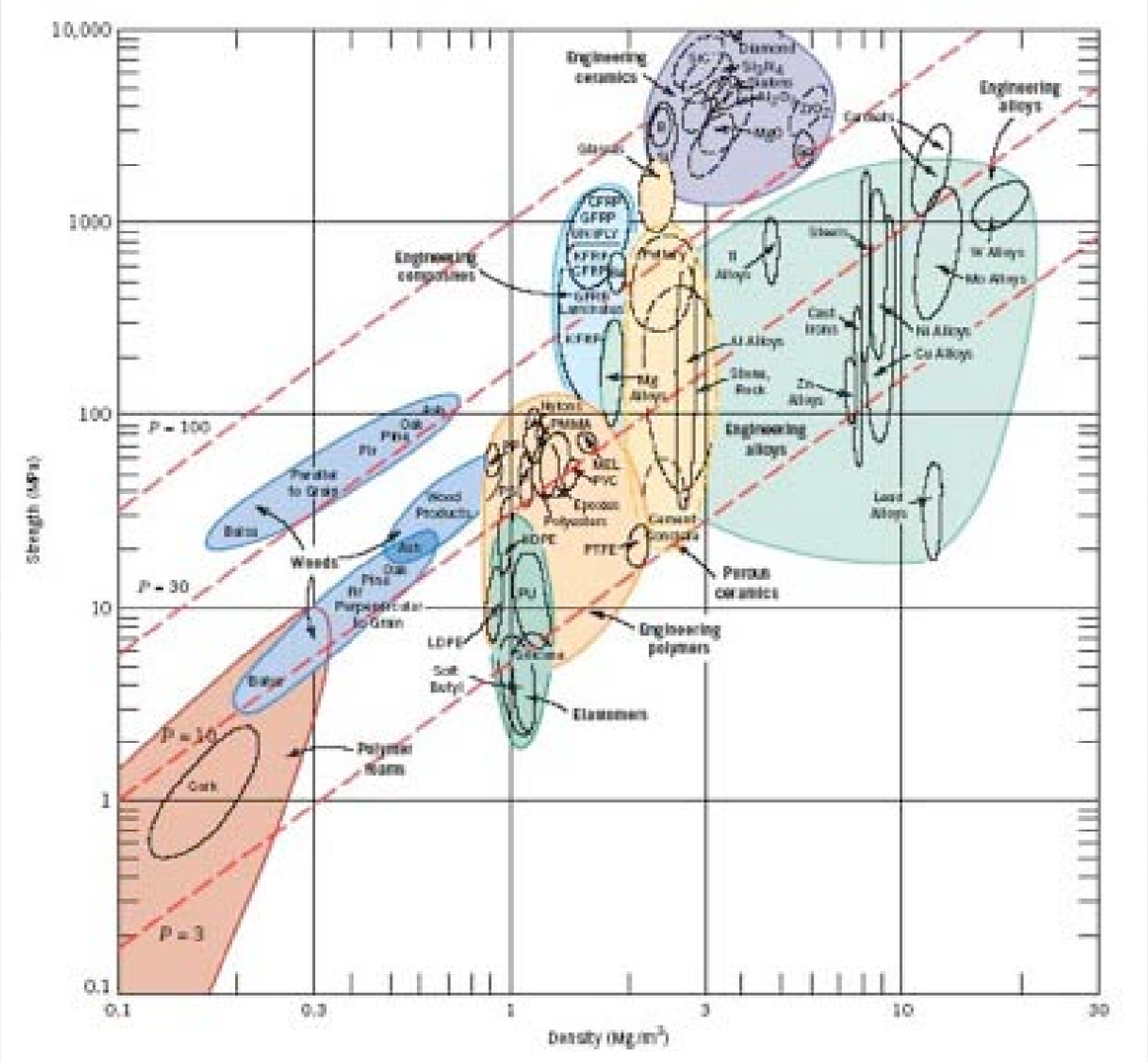
Ames Laboratory

throughout history, humans have been very good at using materials without having a clear understanding of what causes their behavior

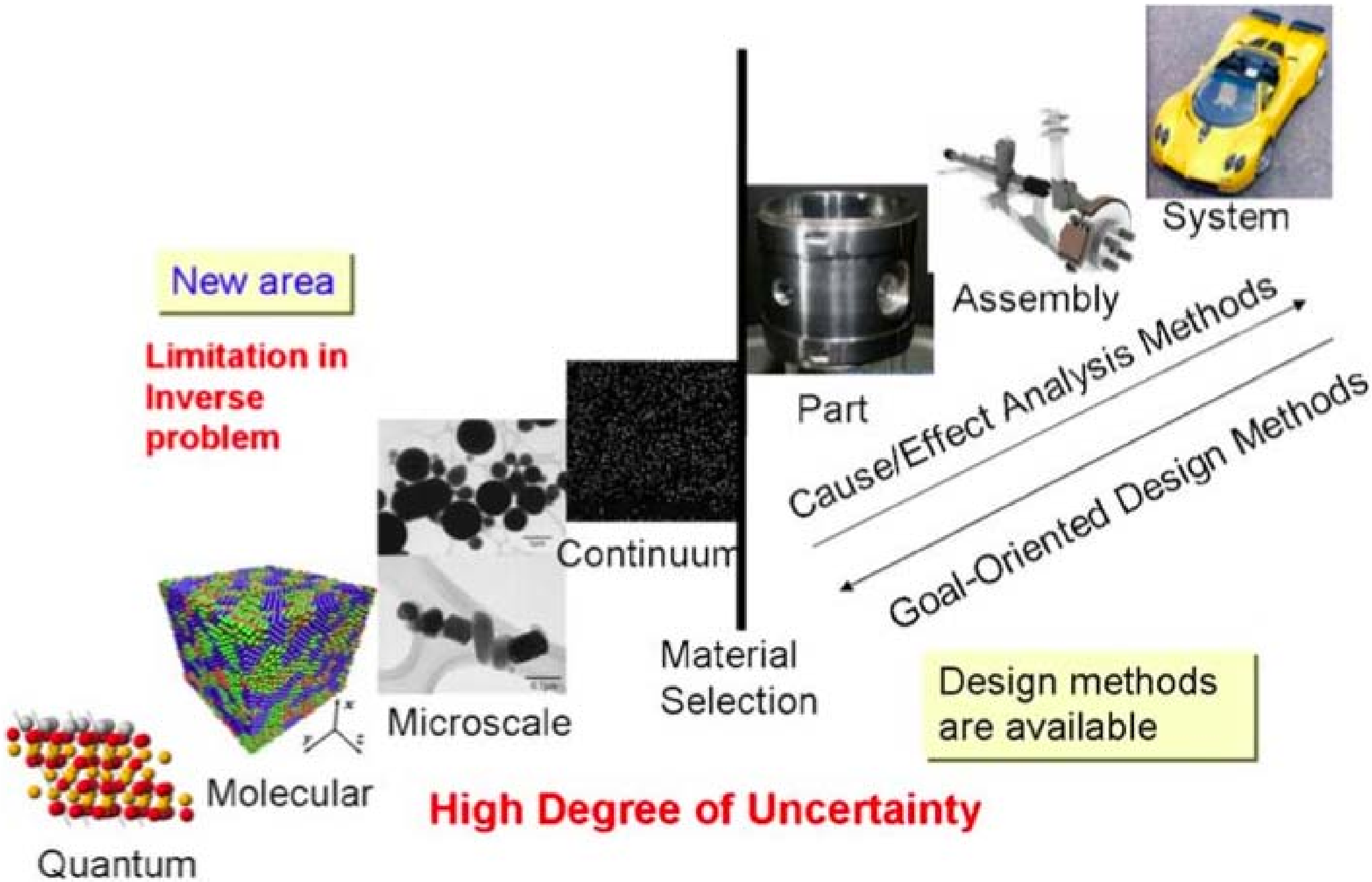
the situation has not really changed very much when it comes to designing products

the materials engineer does materials selection not materials *design*



we need to design the materials concurrently with the design of a product

concurrent design of products

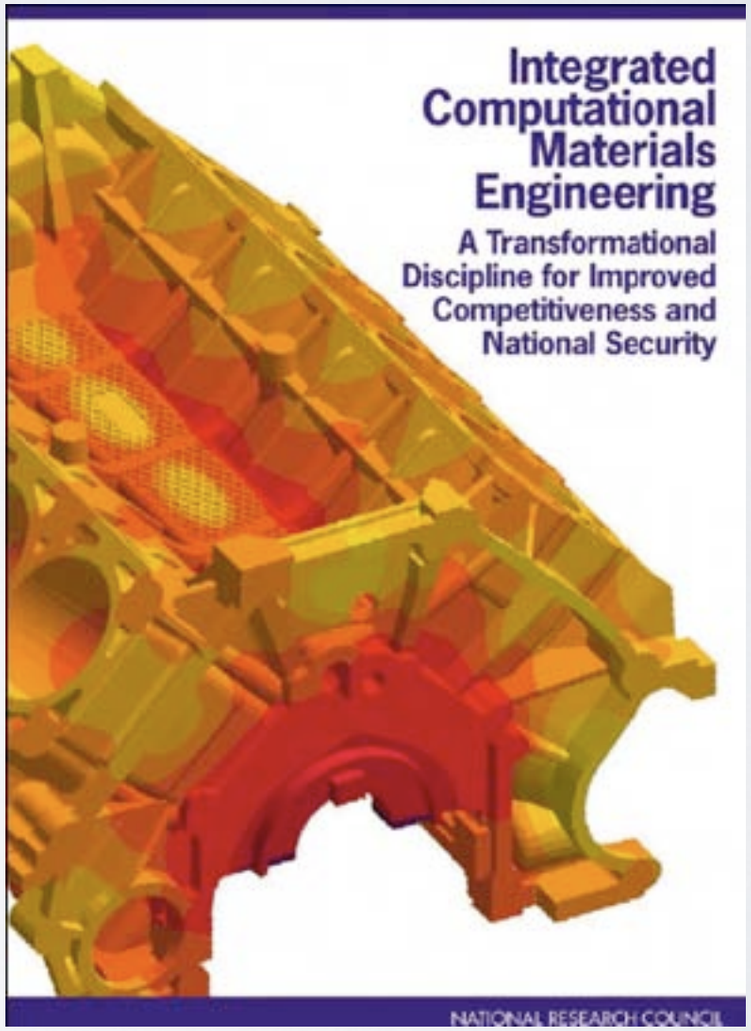


from D. L. McDowell and G. B. Olson, *Concurrent design of hierarchical materials and structures*, Sci. Model Simul. 15, 207 (2008)

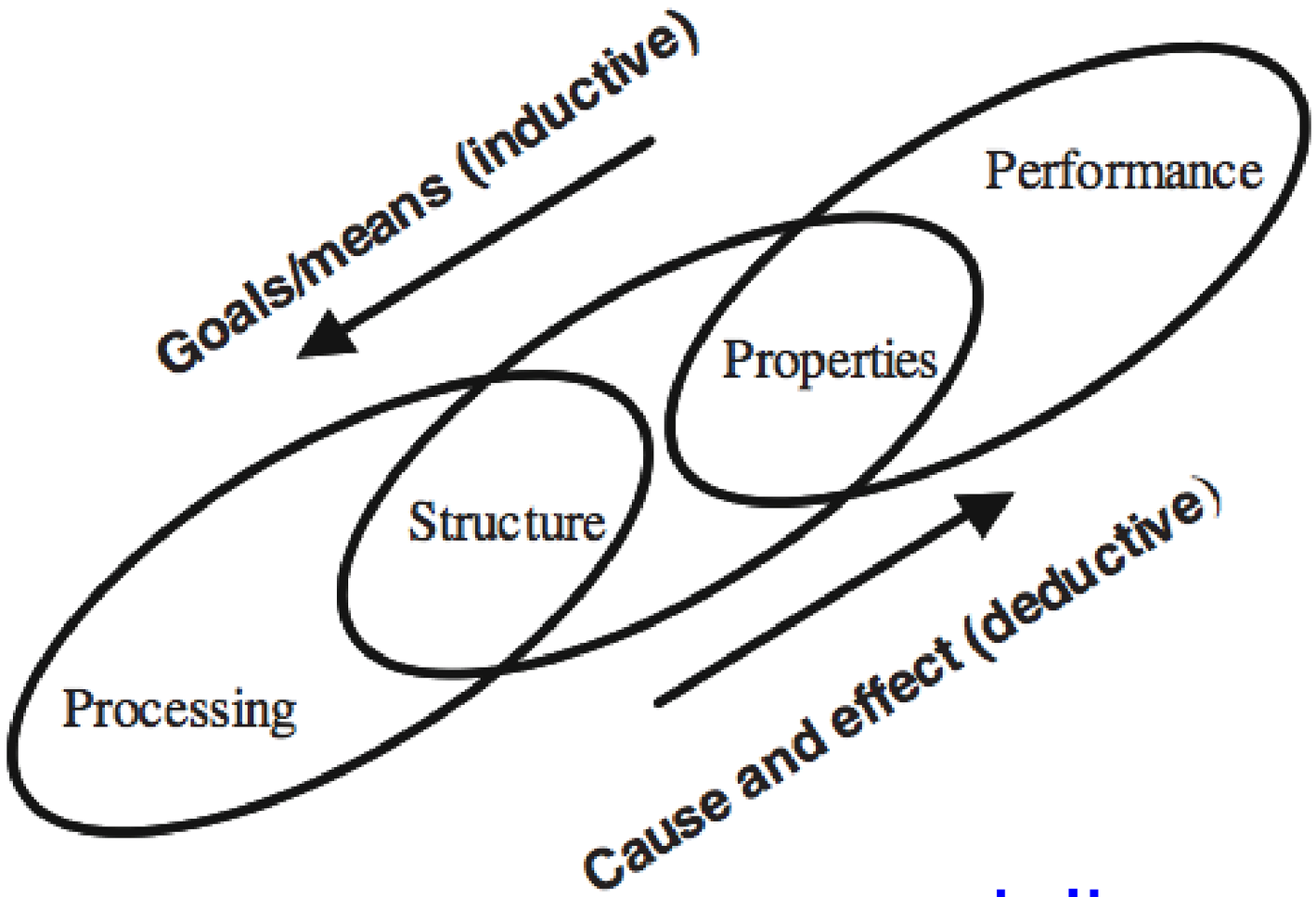
Integrated Computational Materials Engineering

U. S. National Academies

study sponsored by
DoD, DOE/NNSA,
DOE/EERE



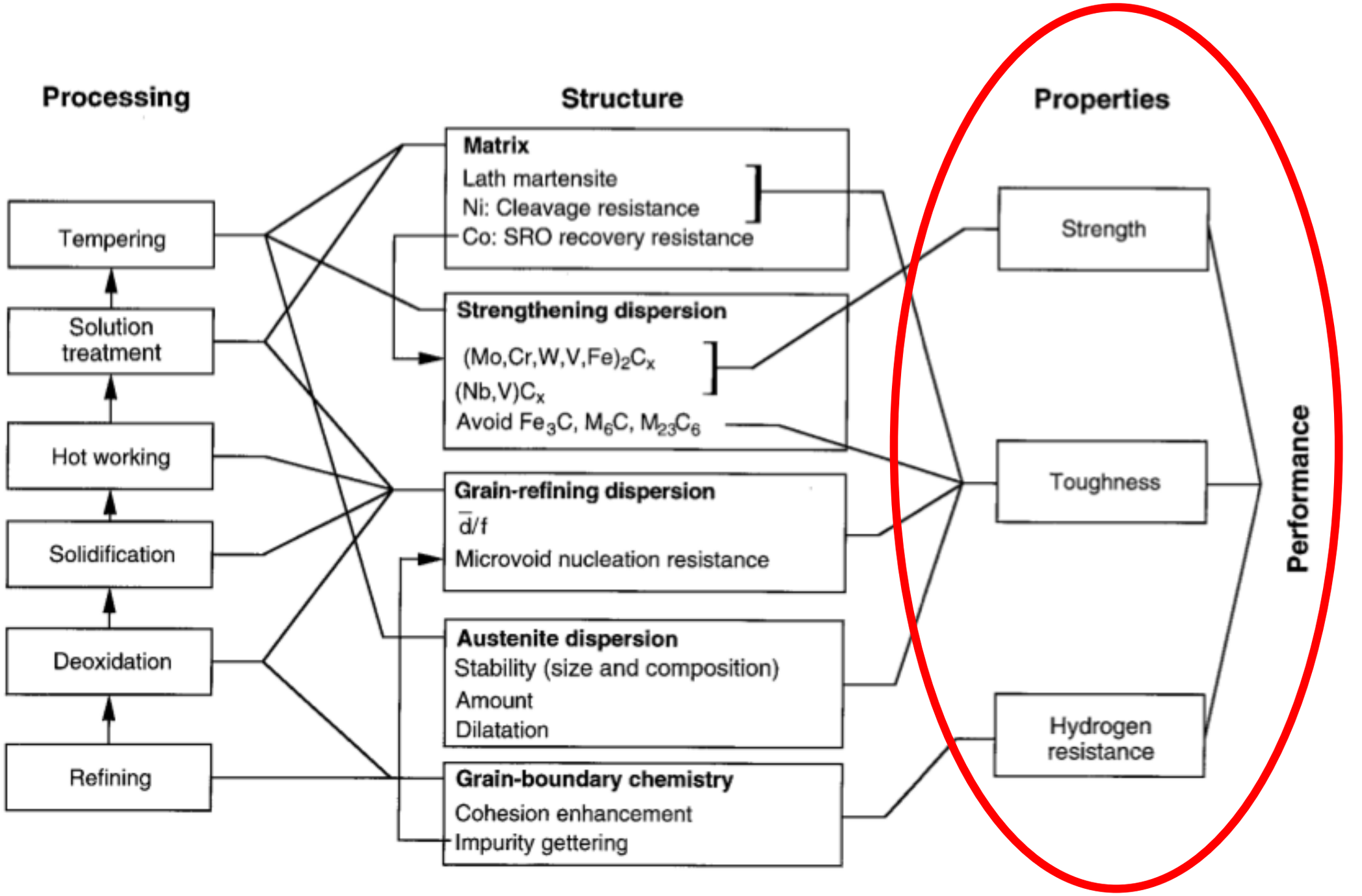
materials design requires a link between science and engineering that is now lacking



modeling and simulation offers us an opportunity to create that linkage

from G. B. Olson, *Computational Design of Hierarchically Structured Materials*, Science 277, 1237 (1998)

processing to properties



materials selection

from G. B. Olson, *Computational Design of Hierarchically Structured Materials*, Science 277, 1237 (1998)

materials design is not ...

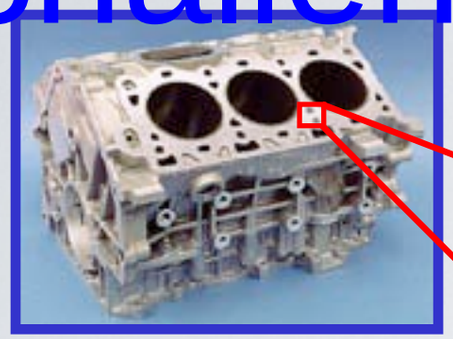
- materials selection
- computational materials science or multiscale modeling
- materials informatics
- just modeling and simulation
- a replacement for all experiments
- either completely intuitive or completely automated
- ...

as in all design processes, materials design requires human decision making

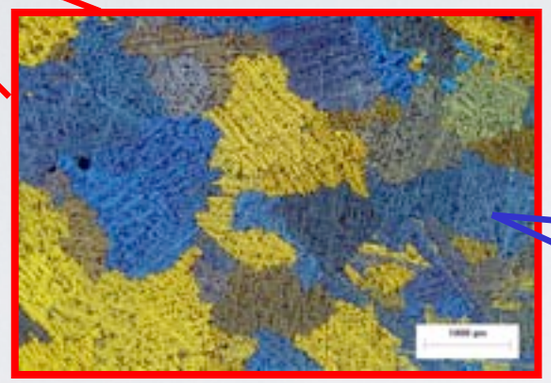
the goal of our program is to create a computational space to facilitate those decisions

the materials challenge

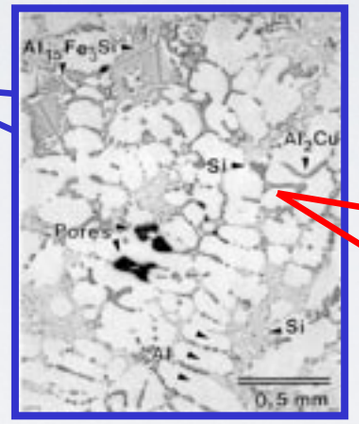
multiple and coupled phenomena acting across an enormous range of length and time scales



Engine Block
≅1 meter

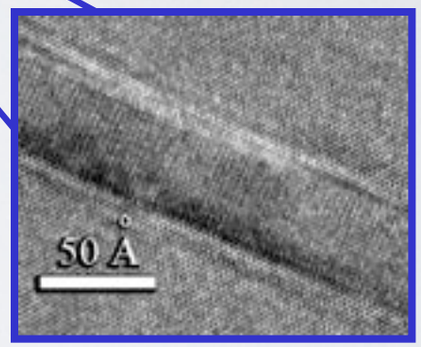


Microstructure
- Grains
≅ 1 – 10 mm
Properties
- **High cycle fatigue**
- **Ductility**



Microstructure
- Phases
≅100 – 500 microns
Properties
- **Yield strength**
- **Ultimate tensile strength**
- **High cycle fatigue**
- **Low cycle fatigue**
- **Thermal Growth**
- **Ductility**

Microstructure
- Phases
≅ 3-100 nanometers
Properties
- **Yield strength**
- **Ultimate tensile strength**
- **Low cycle fatigue**
- **Ductility**



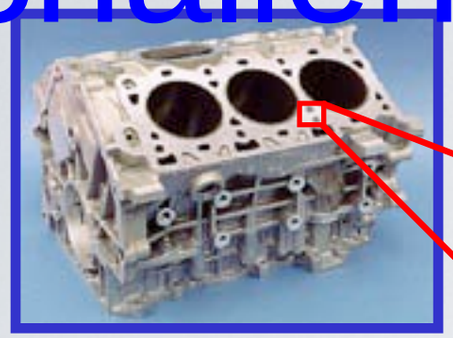
Atoms
≅10-100 Angstroms
Properties
- **Thermal Growth**
- **Yield Strength**

there is a spectrum of relaxation times for these processes - materials are not in equilibrium - properties are path dependent

slide courtesy of J. Allison, Ford (now U. Michigan)

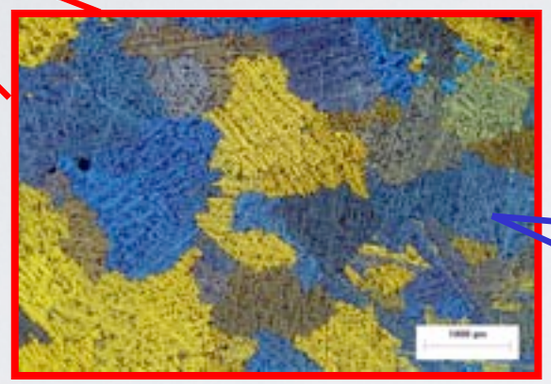
the modeling challenge

the key question is how information is passed across scales



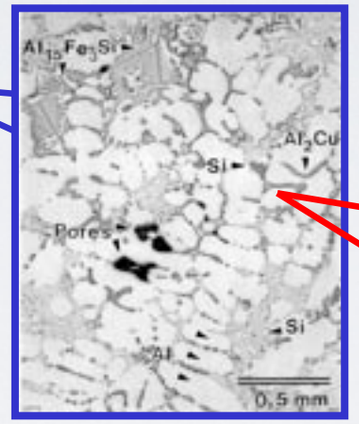
Engine Block
≅1 meter

finite-element methods, heat transfer methods, ...



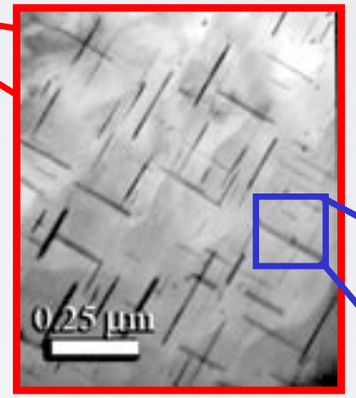
Microstructure - Grains
≅ 1 – 10 mm

phase-field, polycrystal plasticity finite-element methods, ...



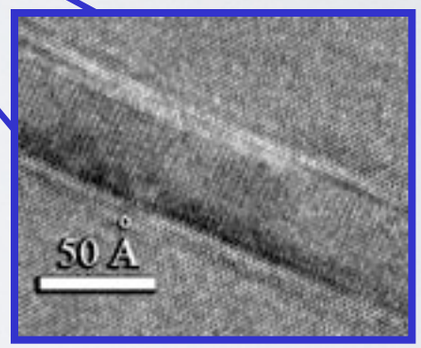
Microstructure - Phases
≅100 – 500 microns

phase-field methods, thermodynamic methods, dislocation dynamics micromechanics, ...



Microstructure - Phases
≅ 3-100 nm

atomistics, phase-field methods, thermodynamic methods, dislocation dynamics, ...



Atoms
≅10-100 Å

electronic structure methods, atomistic simulations

modeling at each level is based on different methods and ***often done by different groups***

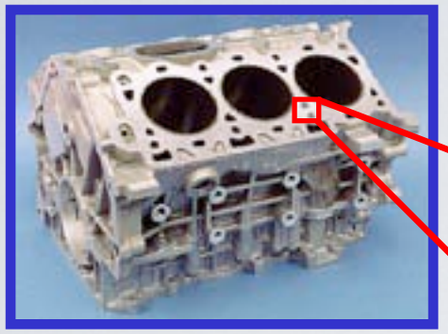
slide based on one from J. Allison, Ford (now U. Michigan)

the usual approach to multiscale simulations

- assume a sequential linkage of “boxes” between atoms and the continuum
- information is passed from one box to the next - “message passing” or a “handshake”

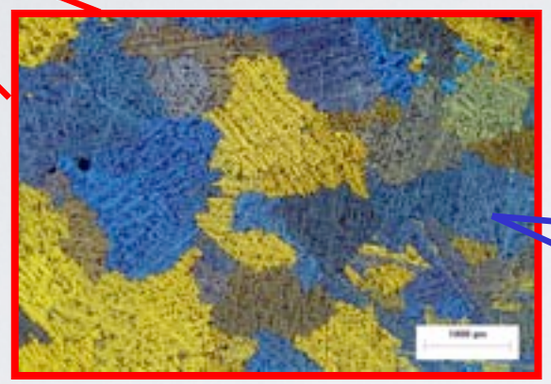
“message passing”

data (from simulations or experiments) at each scale are “averaged”, providing models for next larger scale



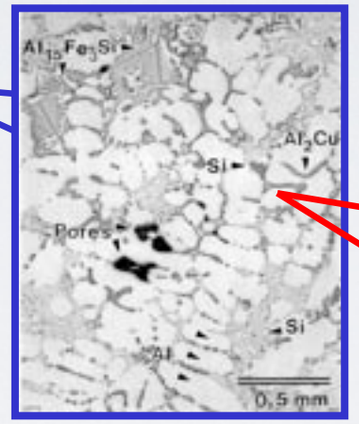
Engine Block
≅1 meter

finite-element methods, heat transfer methods, ...



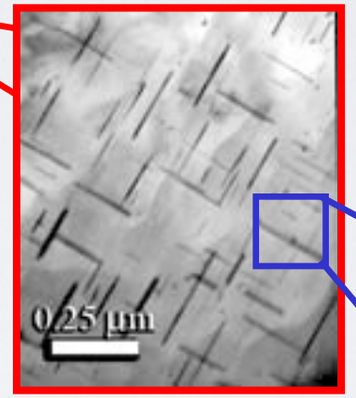
Microstructure - Grains
≅ 1 – 10 mm

phase-field, polycrystal plasticity finite-element methods, ...



Microstructure - Phases
≅100 – 500 microns

phase-field methods, thermodynamic methods, dislocation dynamics micromechanics, ...



Microstructure - Phases
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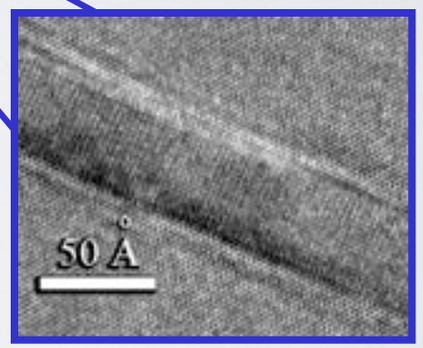
atomistics, phase-field methods, thermodynamic methods, dislocation dynamics, ...



Atoms
≅10-100 Å

electronic structure methods, atomistic simulations

works well for many problems: the Ford virtual casting project

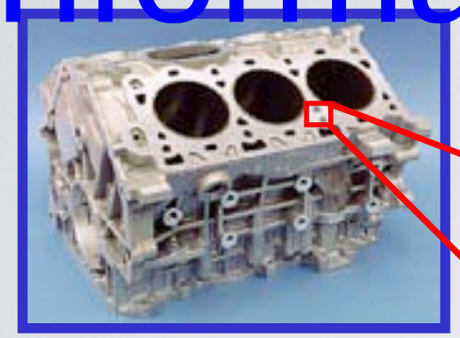
slide based on one from J. Allison, Ford (now U. Michigan)

some issues with the “message passing” approach

- wasteful of information
- ignores non-linearities and overlap of scales
- often lack the “inverse” models to go down in scales

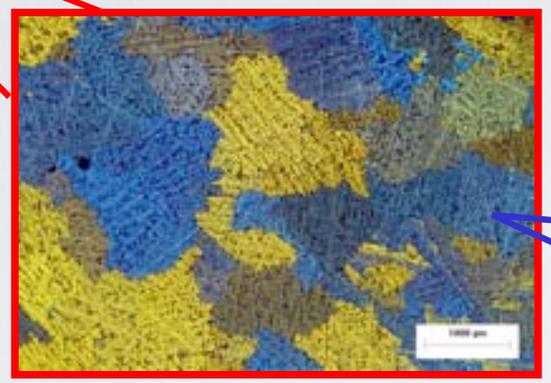
wasting information

homogenization may require multiple simulations (or experiments), with most of the information not really needed



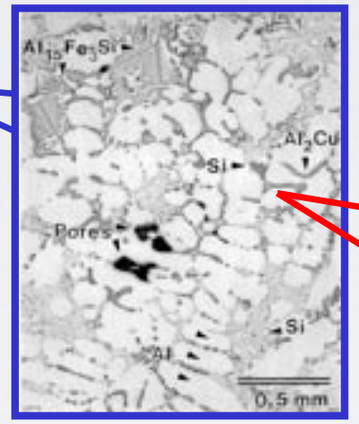
Engine Block ≅1 meter

finite-element methods, heat transfer methods, ...



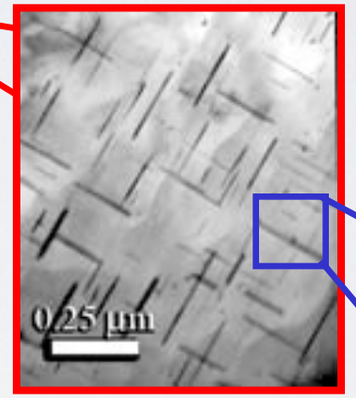
Microstructure - Grains ≅ 1 – 10 mm

phase-field, polycrystal plasticity finite-element methods, ...



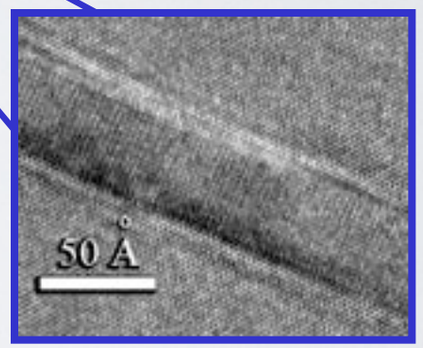
Microstructure - Phases ≅100 – 500 microns

phase-field methods, thermodynamic methods, dislocation dynamics micromechanics, ...



Microstructure - Phases ≅ 3-100 nm

atomistics, phase-field methods, thermodynamic methods, dislocation dynamics, ...



Atoms ≅10-100 Å

electronic structure methods, atomistic simulations

e.g., atoms to dislocations: most atoms in simulation not involved or much influenced by the dislocations

slide based on one from J. Allison, Ford (now U. Michigan)

information across scales

- the vast majority of variables have an information value of zero so we should avoid wasting time considering them
- the problem is that we often do not know which variables have high information value
- we try to avoid that problem by using reduced-order models, but when we do that, we introduce uncertainties

uncertainty and risk

uncertainty is the lack of complete certainty(characterized by a set of probabilities assigned to a set of possibilities)

risk is a state of uncertainty in which some of the possibilities involve a loss, catastrophe, or other undesirable outcome (characterized by a set of possibilities each with quantified probabilities and quantified losses)

uncertainty only matters if there is risk

what is needed

- advances in models and experiments
- information science: theory, databases, informatics, advanced visualization, ...
- multiscale information management
- decision science for concurrent engineering

adapted from D. L. McDowell and G. B. Olson, *Concurrent design of hierarchical materials and structures*, Sci. Model Simul. 15, 207 (2008)

as in all design processes, materials design requires human decision making

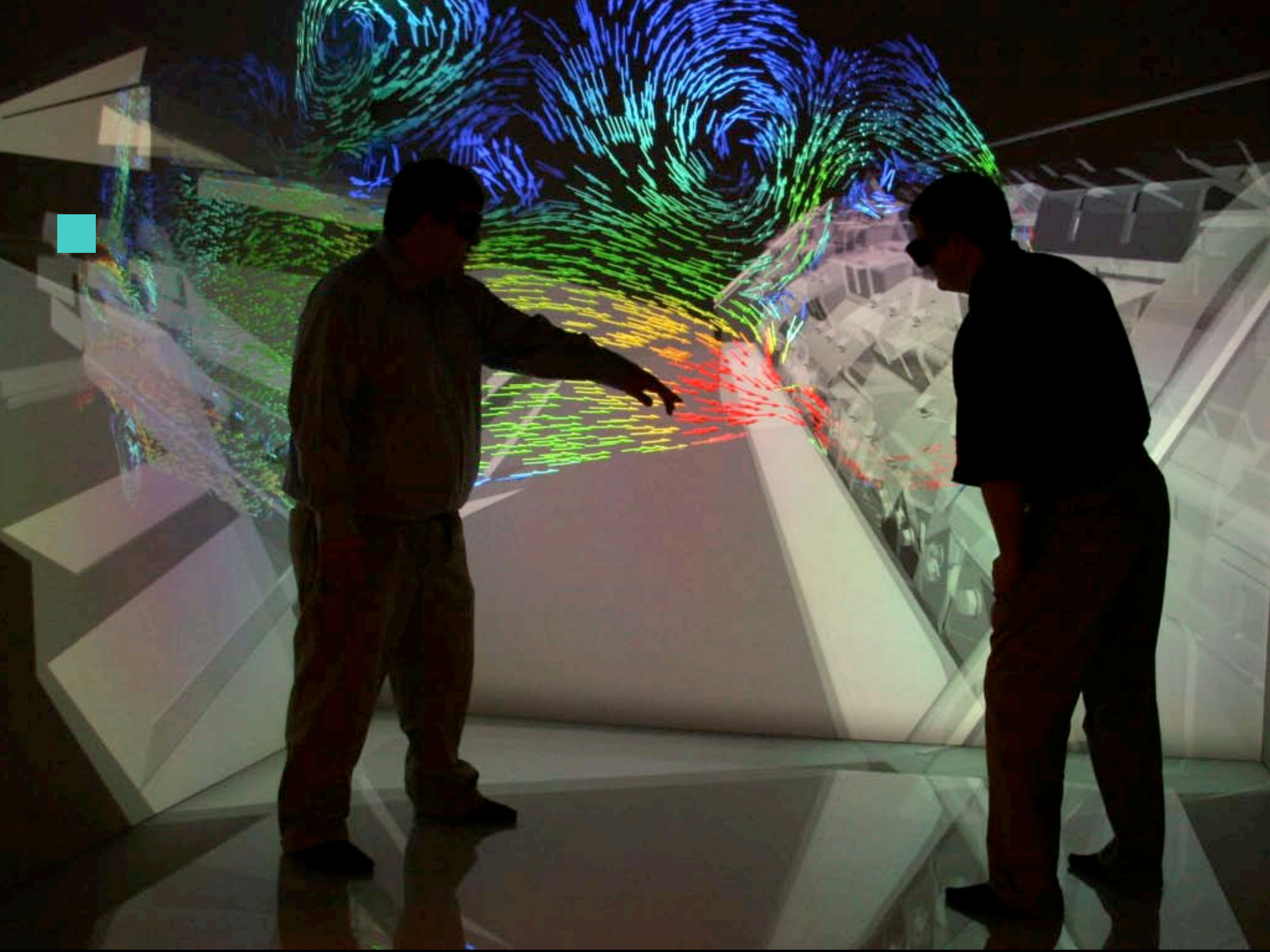
the goal of our program is to create a computational space to facilitate those decisions

VE-Suite:

Creating a common decision space

We are seeking ...

A simple, straight forward way to create, explore, and understand the integrated computational environments (ICE) that represent complexity of systems in our world



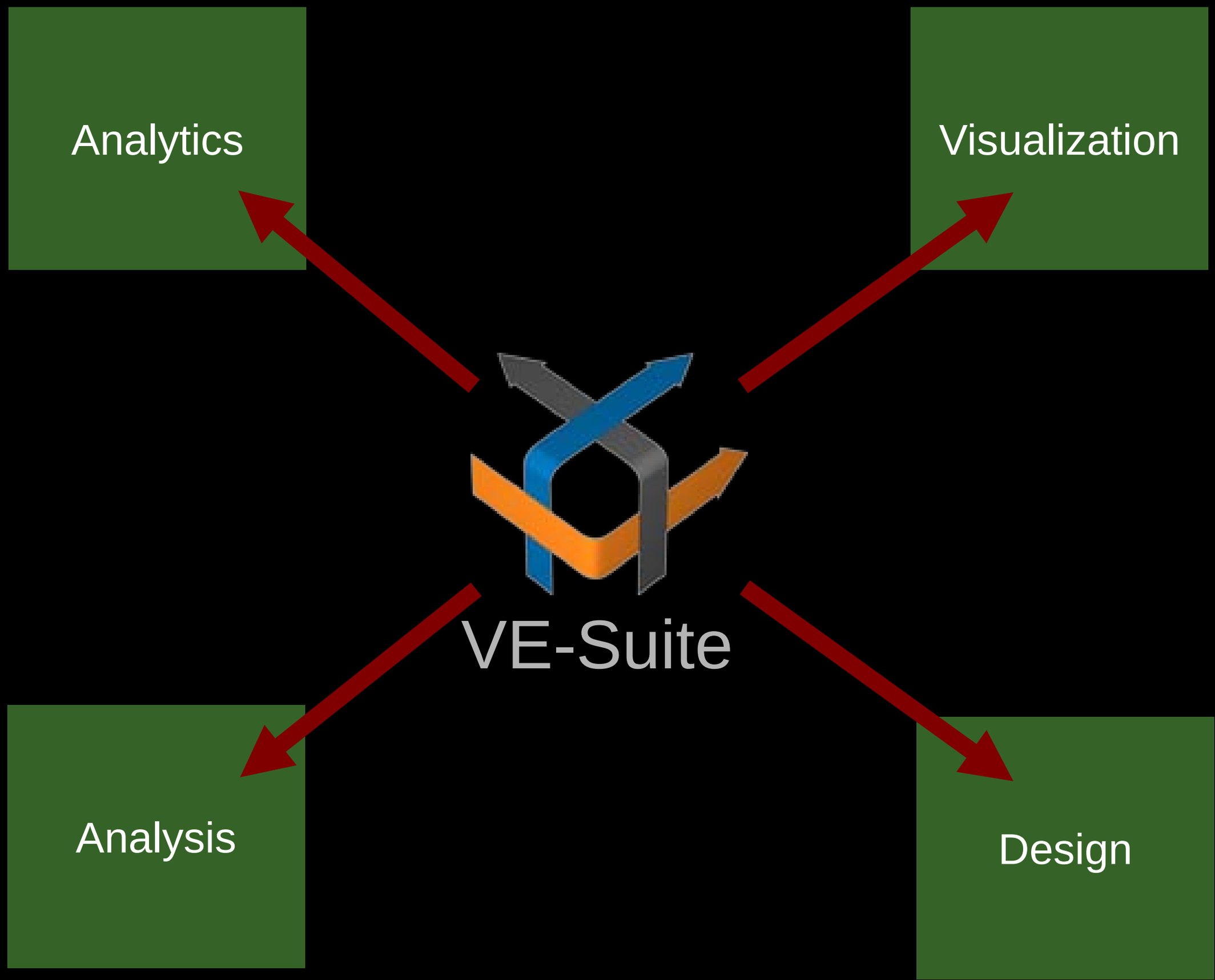
National Excellence in Technology Transfer Award

2009

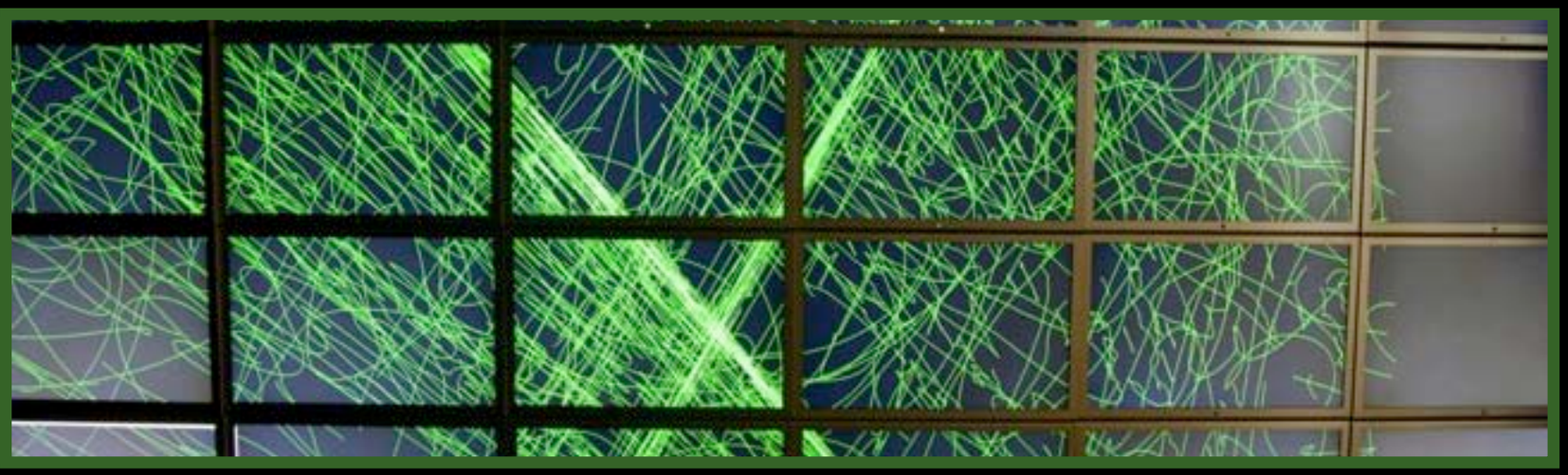
2006

2009

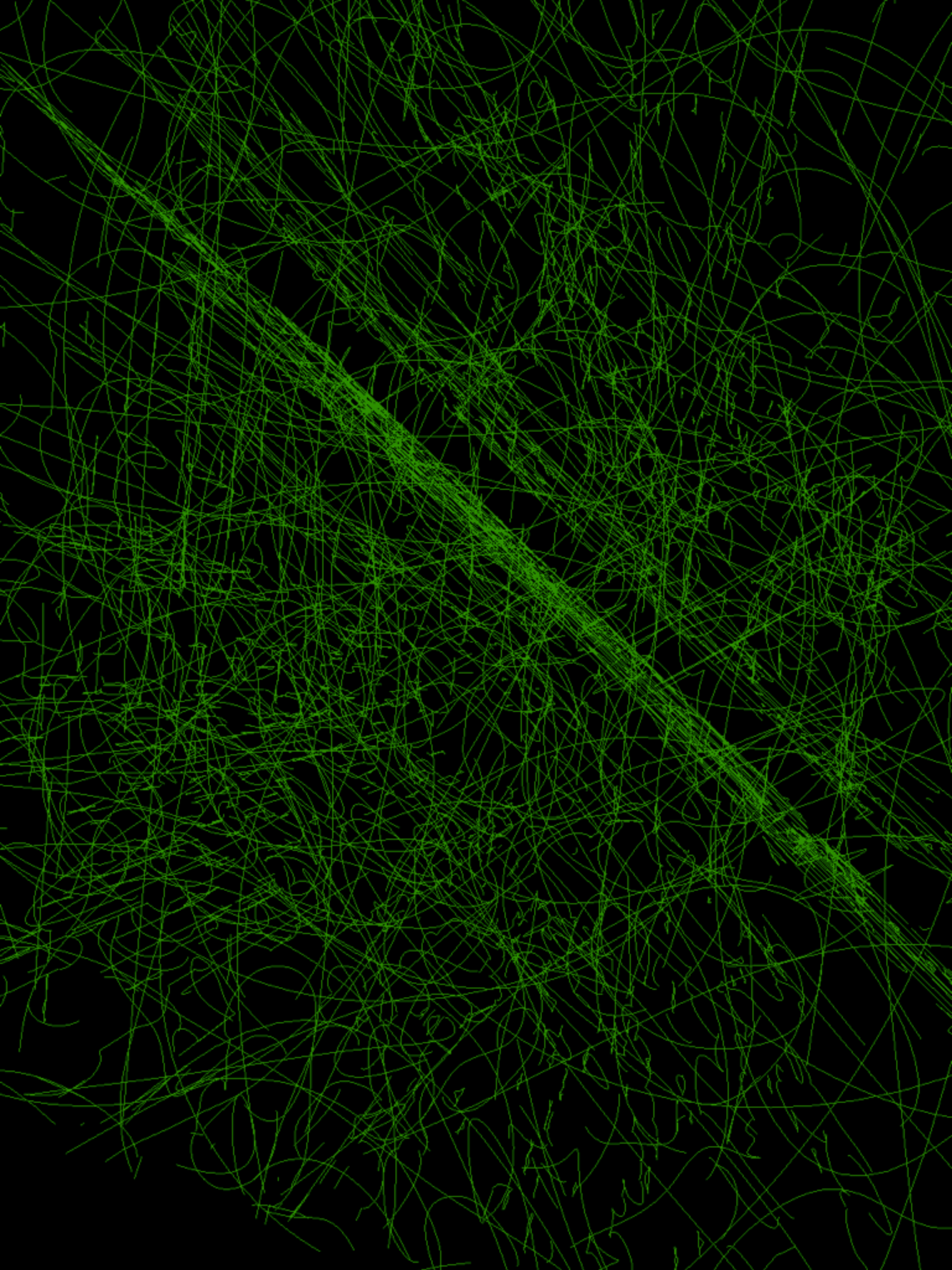
2010


Analytics
Visualization
VE-Suite
Analysis
Design

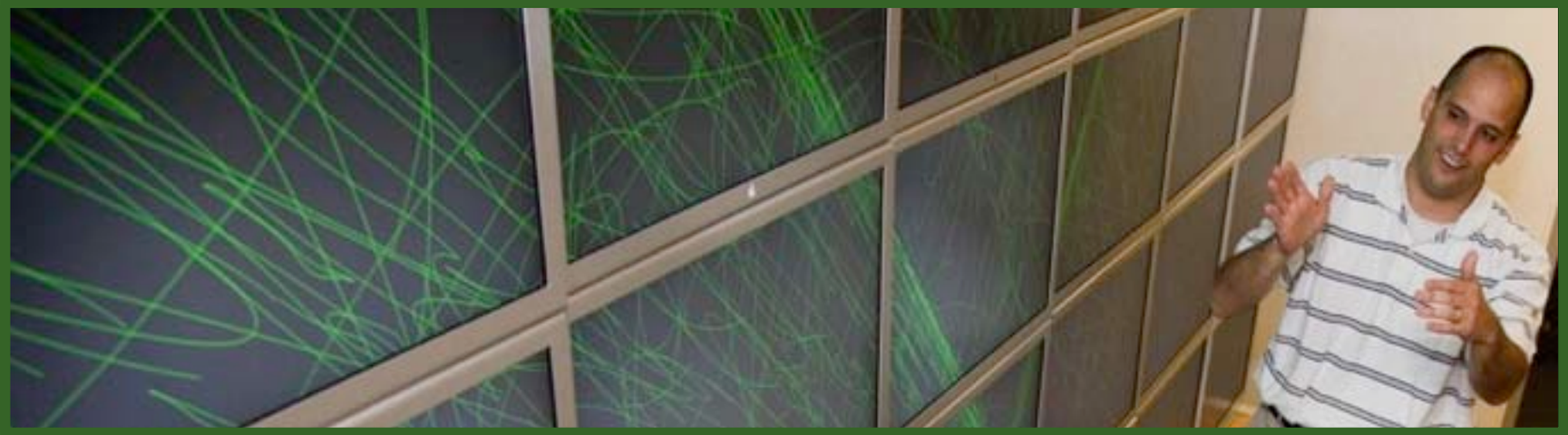
Visualization



- 100+ million points
- Any data source
- Any visualization platform
- Any compute platform
- Realtime sensor visualization

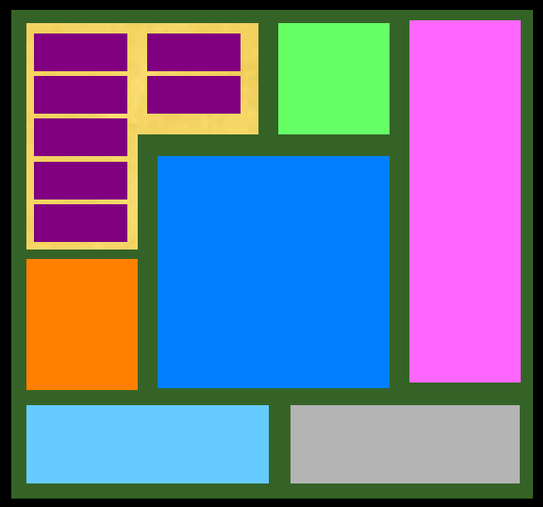


Interaction



- Realtime interaction
- Any user interface
- Physics engine (interferences)
- Information management
- Interactive design and optimization

Integration



Fluent

StarCD

Ensight

ABAQUS

ANSYS

ProE

JT

AutoCad

Bentley

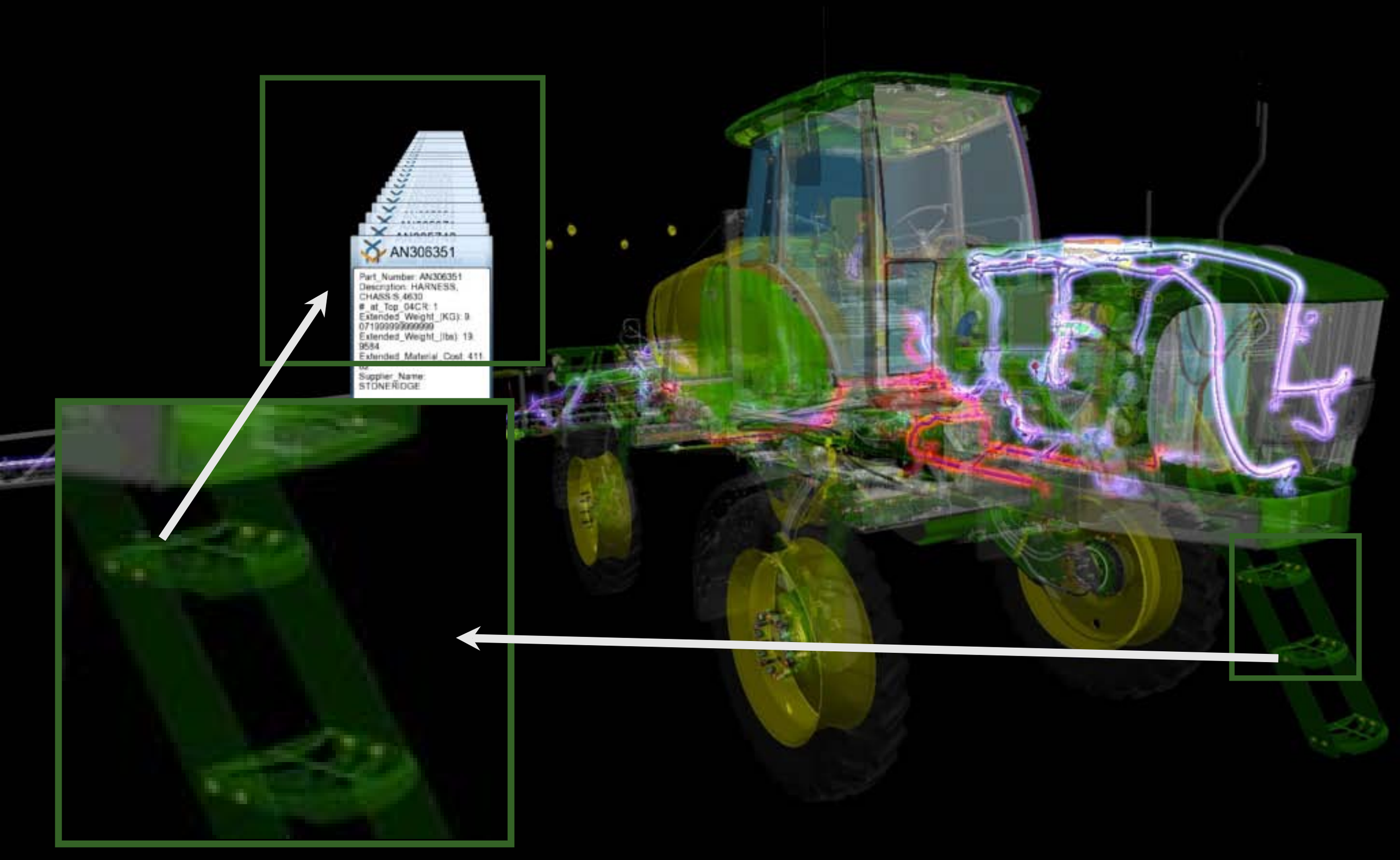
MSC/Patran

Aspen

DynSim

MSC/NASTRAN

...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STONERIDGE

Multiscale

Current modeling approaches

- Phenomenological
- Reduced order model
- Direct Homogenization

Message passing & handshakes

- Codes at different scales are created by different “tribes”
- We manage numbers not information
- Enormous computing needs

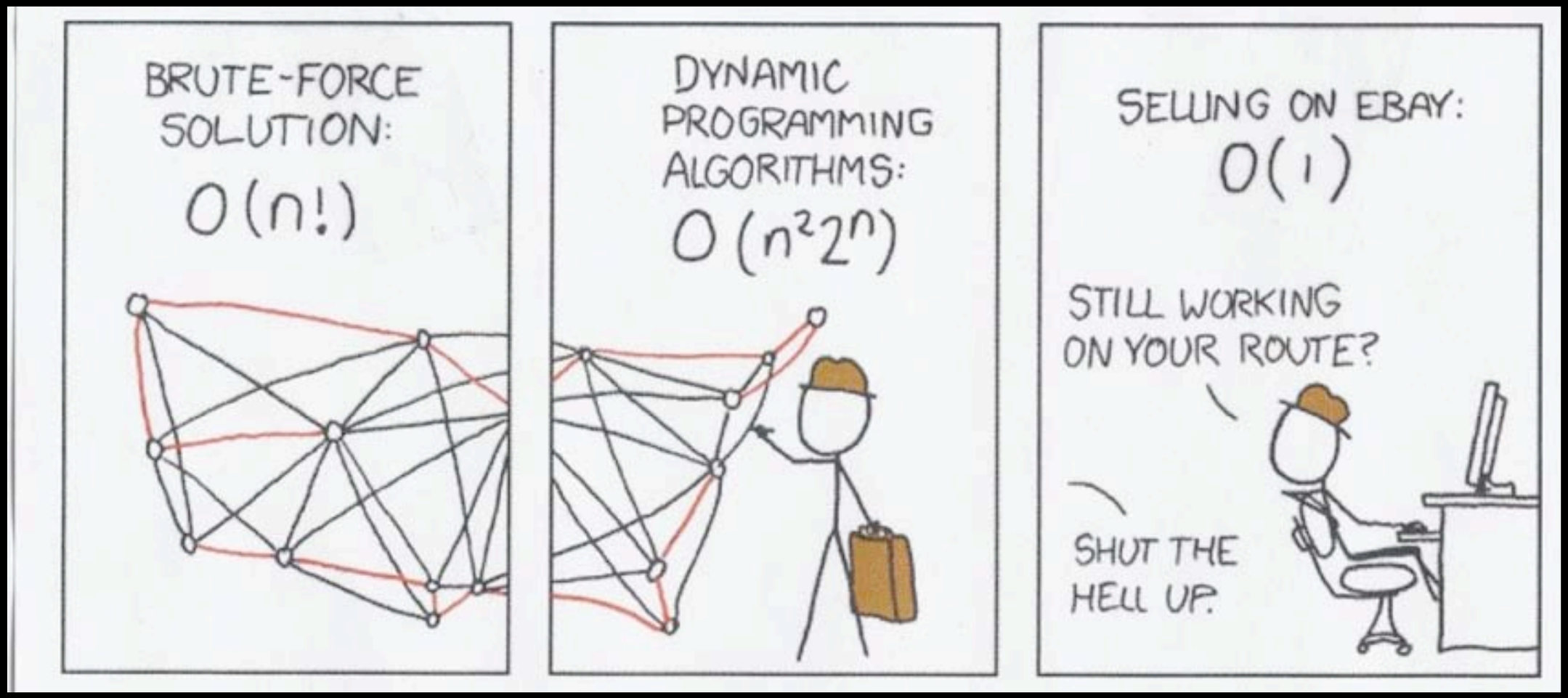
Today we cannot model the richness, fullness, or complexity of engineered, human, or natural systems.

These problems are process rich ...

.... but our current models are process poor

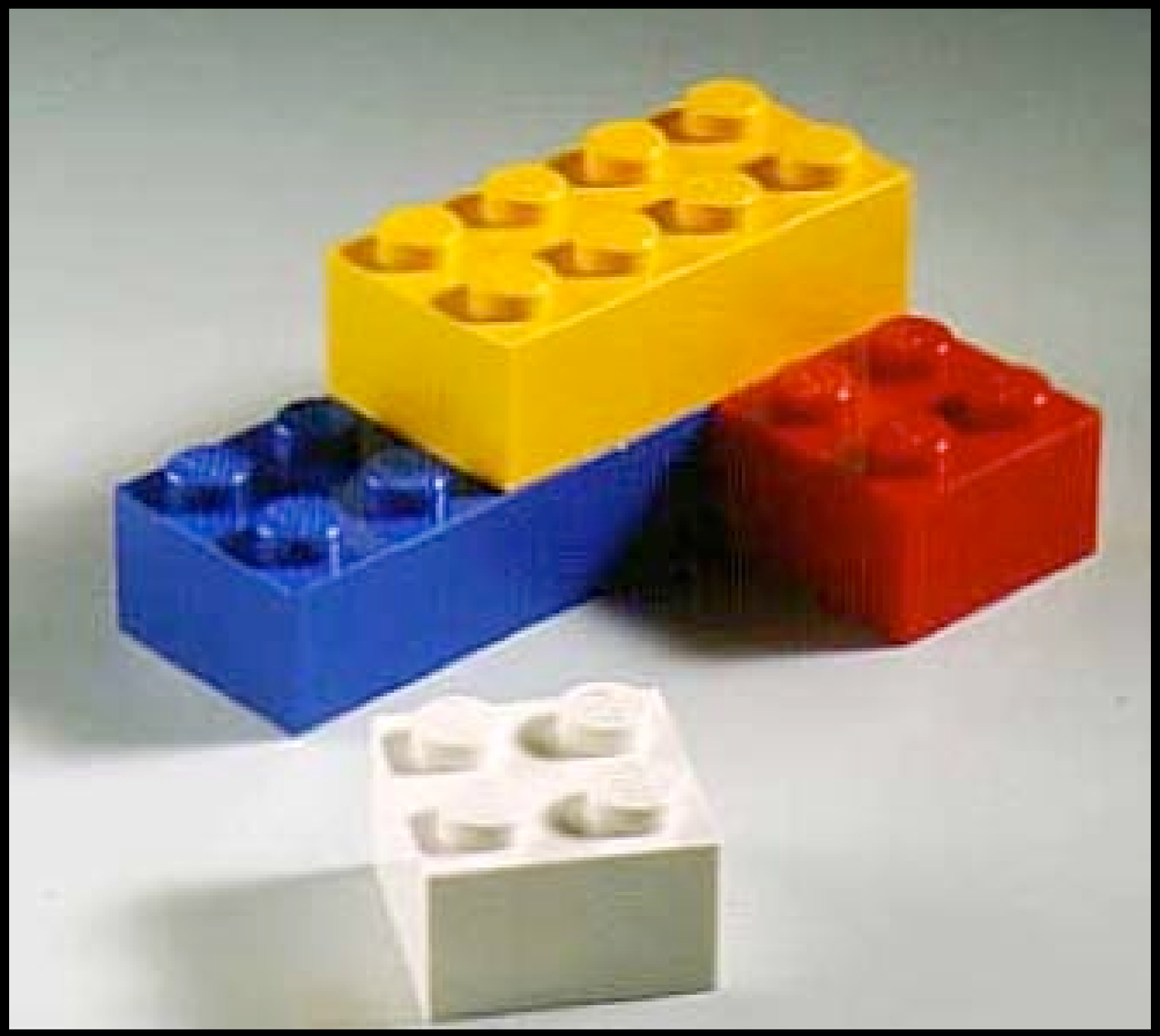
Process rich?

- Coupled linkage across scales
- Coupled linkage across systems
- Self organization & emergence
- Complexity

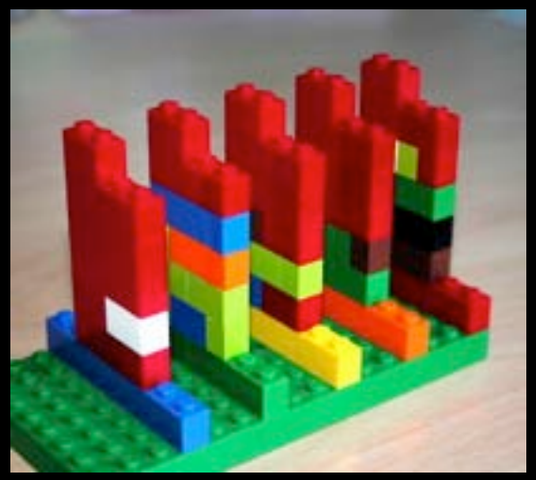


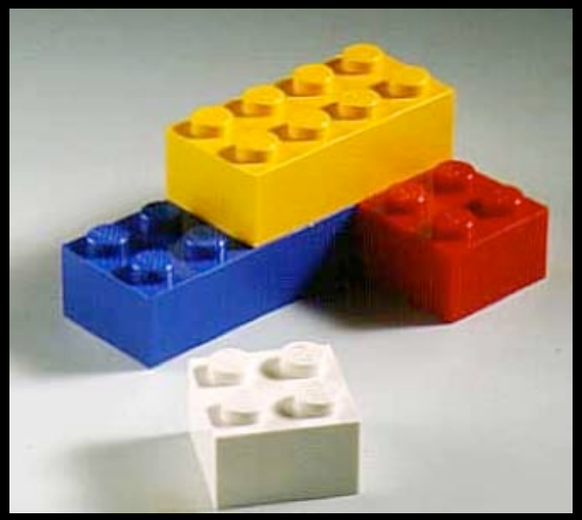
The traveling salesman problem

Our approach



Building Blocks
(objects)



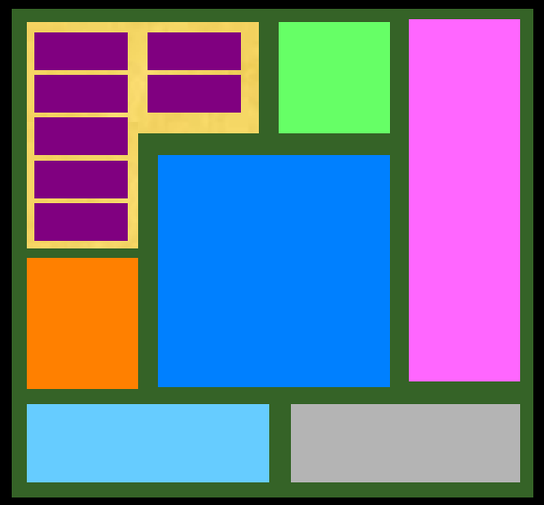


Fully coupled, complex system management

- Sparse matrix theory
- Hierarchical networks
- Combinatorial graphs
- Information theory

Create an object (block)

- Models and information to be linked
- Define coupliing
- Define common “spatial” frame
- Define information needs



Create an object of objects

- Blocks and information to be linked
- Define coupliing
- Define common “spatial” frame
- Define information needs

Repeat

- …
- …
- …
- …

Computational object

$$\underbrace{\begin{bmatrix} A_{1,1} & \cdots & \cdots & \cdots & A_{1,n} \\ \vdots & \ddots & & & \vdots \\ \vdots & & \ddots & & \vdots \\ \vdots & & & \ddots & \vdots \\ A_{n,1} & \cdots & \cdots & \cdots & A_{n,n} \end{bmatrix}}_{\overline{\overline{\mathbf{A}}}} \underbrace{\begin{bmatrix} x_1 \\ \vdots \\ \vdots \\ \vdots \\ x_n \end{bmatrix}}_{\overline{\mathbf{x}}} = \underbrace{\begin{bmatrix} B_1 \\ \vdots \\ \vdots \\ \vdots \\ B_n \end{bmatrix}}_{\overline{\mathbf{B}}}$$

An object composed of objects

$$
\begin{bmatrix}
\begin{bmatrix} [\cdots] & [\cdots] \\ [\cdots] & [\cdots] \end{bmatrix} & [\cdots] & [\cdots] \\
[\cdots] & \begin{bmatrix}
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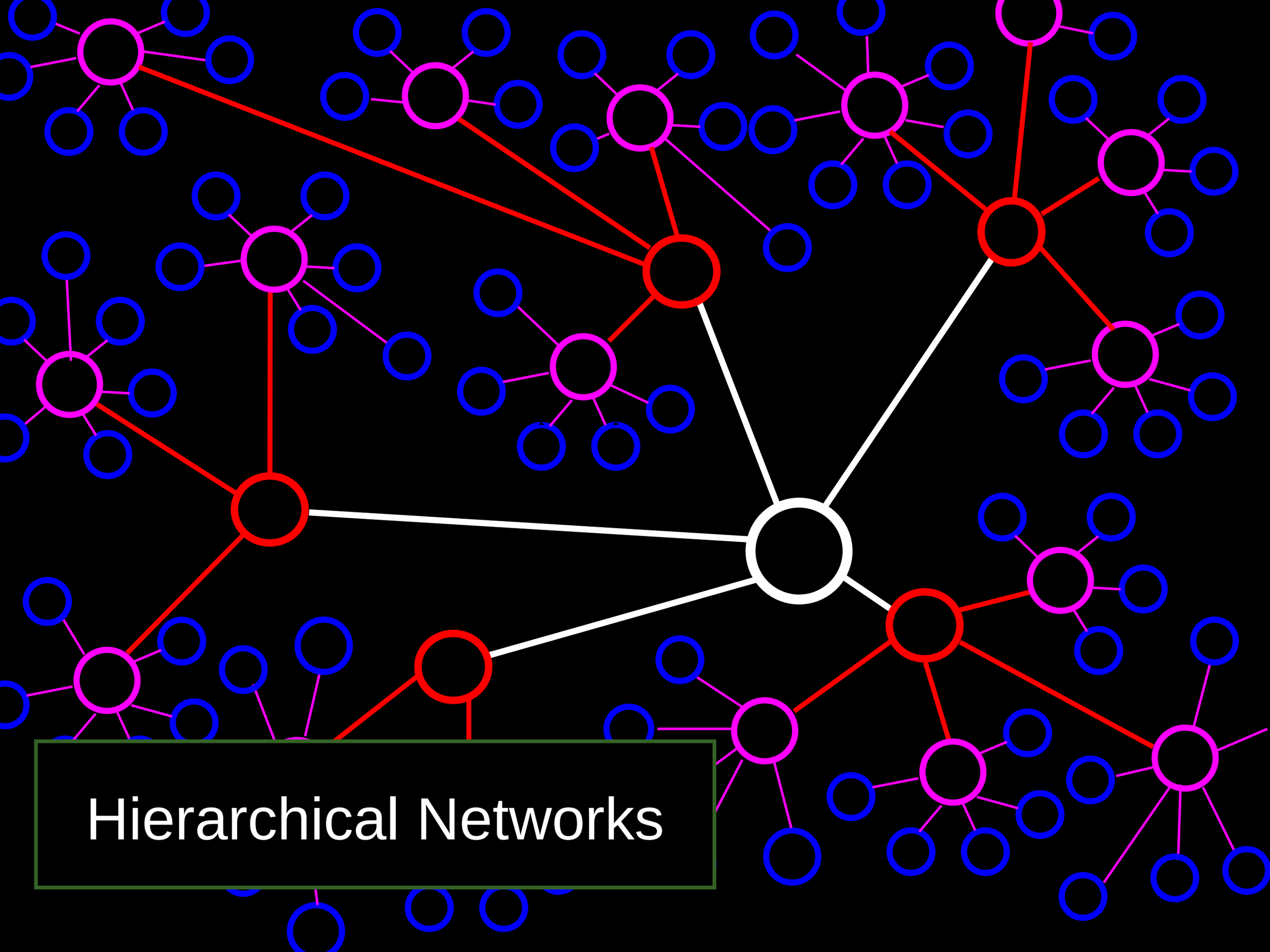
[\cdots] & [\cdots] & [\cdots] & [\cdots] \\
[\cdots] & [\cdots] & [\cdots] & [\cdots]
\end{bmatrix} & [\cdots] \\
[\cdots] & [\cdots] & \begin{bmatrix} [\cdots] & [\cdots] \\ [\cdots] & [\cdots] \end{bmatrix}
\end{bmatrix}
$$

Linkage/Coupling

- Direct (the old way)
- Orthogonal decomposition
- Adaptive blocks modeling
- Coupled neural network, general regression neural network
- ... others

Computing in the cloud



Hierarchical Networks

We are working in the emerging intersection between information, computation, and complexity

MIT Media Lab ...

“... one of the world’s top computing science laboratories”

New York Times, April 26, 2011

We are seeking ...

A simple, straight forward way to create, explore, and understand the integrated computational environments (ICE) that represent complexity of systems in our world

MULTISCALE DESIGN LABORATORY

- have state-of-the-art graphics including a high resolution wall and 3D visualization
- a physical space in which designers, materials scientists, etc. can collaborate